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# QUASI ONE-DIMENSIONAL STEADY-STATE MODELS FOR GAS LEAKAGE - PART II: IMPROVEMENT OF THE VISCOUS MODELING

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## ABSTRACT

A comparison between four quasi one-dimensional steady-state gas leakage models, presented in a parallel paper, showed that none of them proved to be satisfactory. The results suggest that the modeling of the wall shear stress is the main flaw in the models. By fitting the shear stress to experimental data, an attempt was made to find a more acceptable model. For this a flow model was combined with an optimization algorithm. A second set of experimental data was used to validate the results. The optimized model gives a much better prediction for the set of experimental data used in the optimization. Application of the new model to another, quite different set of experimental data shows a slight improvement in comparison to the original. This gives some confidence in the improvement. Simulations show that choking, and thereby the occurrence of shock waves, is a realistic possibility in leakage.

## INTRODUCTION

One of the conclusions of a parallel paper [4] was that the modeling of viscous effects, more specific the wall shear stress, in one dimensional leakage models is poor. As a logical follow up, optimization of the wall shear stress computation was attempted. Of the two sets of experimental data that were already used in the parallel paper, those by Peveling were used for the optimization, Ishii's for validation. Since these apply to quite different conditions (air/R22, clearance heights 100..500/10  $\mu\text{m}$ , pressure ratio's 1.2..2.2/1..15 respectively), good prediction of the data which were not used in the optimization increases the confidence in the results.

For the optimization a quasi one-dimensional steady state model was combined with an optimization algorithm. The model by Xiuling (see parallel paper) was selected because it showed good qualitative behavior and proved to be numerically stable. The investigation presented here seeks to improve its quantitative predictions. Because derivatives of the object function, *ie.* the function that is actually optimized, cannot be found in an effective way, the selection of the optimization algorithm was first narrowed down to methods that don't need any. Since there are no available criteria for further selection, the Downhill-Simplex method of Nelder & Mead was chosen intuitively, the implementation was taken from Press *et al.* [3].

## nomenclature

specific heat ratio	$\gamma$	1
dynamic viscosity	$\eta$	Pa.s
reference viscosity	$\eta_0$	Pa.s
friction coefficient	$\xi$	1
pressure ratio	$\Pi$	1
density	$\rho$	kg/m <sup>3</sup>
wall shear stress	$\tau$	Pa
flow area	$A$	m <sup>2</sup>
velocity of sound	$a$	m/s
hydraulic diameter	$D$	m
Mach number	$M$	1
wetted perimeter	$P$	m
pressure	$p$	Pa
specific gas constant	$R$	J/kg.K
Reynolds number	$Re$	1
specific entropy	$s$	J/kg.K
temperature	$T$	K
normal boiling point	$T_B$	K
reference temperature	$T_0$	K
velocity	$u$	m/s
flow path coordinate	$x$	m

The paper starts off with a discussion of the wall shear stress model, followed by derivation of the flow model and an explanation of the optimization procedure. It closes with a discussion of the results and the conclusions. For a description of the measurements is referred to the parallel paper.

## WALL SHEAR STRESS

The use of semi-empirical formulae for the wall shear stress is widely spread. They usually relate the friction coefficient to the Reynolds number. Best known are the relations of Hagen-Poiseuille (which is purely theoretical

with  $a = 64, b = -1$ ) for laminar flow and Blasius ( $a = 0.3164, b = -1/4$ ) for turbulent flow, which have the following form (see VDI-Wärmeatlas [8]):

$$\tau = \frac{1}{2} \rho \xi u^2 \quad \text{with} \quad \xi = a \cdot \text{Re}^b \quad (1)$$

The Reynolds number is based on the hydraulic diameter ( $D = 4A/P$ ). The formulae are based on incompressible boundary theory and assume a fully developed flow. The first is obviously an incorrect assumption, the second probably is. Nevertheless (eq.1) will be used for an improved model, the parameters  $a$  and  $b$  will be the subject of the optimization. A profound introduction to the theory behind (eq.1) can be found in Kays & Crawford [1].

The dynamic viscosity, which was fitted to a straight line in the parallel paper, is replaced by the more realistic model found in Perry & Chilton [5]:

$$\eta(T) = \eta_0 \left( \frac{T}{T_0} \right)^{3/2} \frac{T_0 + 1.47 \cdot T_B}{T + 1.47 \cdot T_B} \quad (2)$$

In figure 1 the properties of the fluids used in this investigation are tabulated.

	R 22	air	
$\eta_0$	12.00	17.16	$\mu\text{Pa}\cdot\text{s}$
$T_0$	273.15	273.15	K
$T_B$	232	75	K

Figure 1: Coefficients in the viscosity model.

## XIULING'S MODEL FOR THE FLOW

Following the general approach in fluid dynamics, the mathematical model of the flow is based on the three great conservation principles of mass, momentum and energy. In addition a series of constitutional equations is required: in this case the shear stress model (eq.1), the equation of state (caloric perfect gas, thus:  $p = R\rho T$  and  $d\gamma = 0$ ) and the viscosity (eq.2). A model very similar to this one, though derived from the two-dimensional Navier-Stokes equations, was presented by Xiuling *et al.* and later used by Zhen & Zhiming [10]. In this section the model is derived.

### Continuity Equation

The conservation of mass is trivial:

$$\rho u A = \dot{m} \quad \Longleftrightarrow \quad \frac{d\rho}{\rho} = -\frac{du}{u} - \frac{dA}{A} \quad (3)$$

### Energy Equation

Due to the wall friction the isentropic assumption is incorrect, but it seems justified to use it anyway: The comparison between the models of Xiuling and Anderson shows relative little difference (see parallel paper). Both solve the same equations for mass and momentum conservation, but the first employs an isentropic, the second a non-isentropic energy equation. The advantage is that the equation gets a very simple form:

$$p\rho^{-\gamma} = \text{constant} \quad \Longleftrightarrow \quad \frac{dp}{p} = \gamma \frac{d\rho}{\rho} \quad (4)$$

### Momentum Equation

The basic form of the momentum equations is:

$$d(\rho u^2 A) + A dp + \tau P dx = 0$$

The first term can be worked out as:  $d(\rho u^2 A) = \rho u A du + u d(\rho u A)$ , of which the last term vanishes due to (eq.3). Together with (eq.1) this yields:

$$\rho u A du + A dp + \frac{1}{2} \rho \xi u^2 P dx = 0$$

By using (eq.4) to eliminate  $dp$  and (eq.3) to eliminate the  $d\rho/\rho$  it introduces, all independent variables except for  $u$  can be removed from the equation:

$$\rho u A \, du - \gamma p A \left\{ \frac{du}{u} + \frac{dA}{A} \right\} + \frac{1}{2} \rho \xi u^2 P \, dx = 0$$

Division of the entire equation by  $\rho u^2 A$ , introduction of the hydraulic diameter, substitution of the Mach number<sup>1</sup> and rearranging, gives the momentum equation for the velocity:

$$\frac{du}{u} = \frac{1}{M^2 - 1} \left\{ \frac{dA}{A} - \frac{2\xi M^2}{D} dx \right\} \quad (5)$$

At sonic conditions, the first term on the right hand side equals  $1/0$ , which can only be physically correct when the bracketed terms also add up to zero. For leakage flows, which are usually highly viscous, this might not occur (the viscous term exceeds the rate of change of the area). This implies that either instability of the flow forbids a steady state solution or that two dimensional effects, such as expansion waves and oblique shocks, forbid one-dimensional modeling. Since there is no subsonic solution, the flow is still expected to become supersonic and (non-normal) shock-waves are therefore inevitable<sup>2</sup>. It is assumed that subsonic flow upto the transition is not influenced by this flaw, leaving the computation of the mass flow rate intact.

The momentum equation is not used in this form, but converted to an equation for the Mach number. Derivation of the square of the Mach number yields:

$$dM^2 = d \left( \frac{\rho u^2}{\gamma p} \right) = M^2 \left\{ 2 \frac{du}{u} + \frac{d\rho}{\rho} - \frac{dp}{p} \right\}$$

Employing the chain-rule the left hand side is written as  $dM^2 = 2M dM$ . This together with elimination of  $dp/p$  with (eq.4) followed by elimination of  $d\rho/\rho$  with (eq.3) yields:

$$\frac{dM}{M} = \frac{\gamma + 1}{2} \cdot \frac{du}{u} + \frac{\gamma - 1}{2} \cdot \frac{dA}{A} \quad (6)$$

The momentum equation as expressed for  $du/u$  is used as a constitutional equation only. The differential equations for  $d\rho/\rho$ ,  $dp/p$  and  $dM/M$  are the final model equations. Of course it should be possible to use the integral form of the continuity and energy equations, leaving only one differential equation, but this leads to a less stable code. The reason for this is not yet understood.

## BOUNDARY CONDITIONS AND NUMERICAL SOLUTION STRATEGY

The most convenient boundary conditions are the inlet pressure and temperature and outlet pressure. This means that the problem is stated as a two point boundary value problem. Therefore straight forward integration of (eq.3,4,6) is not possible. As an iterative solution strategy the shooting method was adopted:

It is obvious that the inlet Mach number can be bracketed between 0 and 1. Now this interval is narrowed down by trying the intermediate value ( $M = 0.5$ ) with which the flow will be simulated. When the flow chokes, becomes supersonic, the trial must be a maximum value. When it remains subsonic and the outlet pressure exceeds the prescribed value, the viscous effects are too low and thus the trial Mach number is too low. By the same line of reasoning, a maximum value is found when the flow remains subsonic and outlet pressure is lower than prescribed. By repeating this sequence the inlet Mach number can be determined upto any accuracy.

When the flow becomes supersonic, the flow downstream of the sonic point is irrelevant to the mass flow rate. Since comparison with the experimental data is based on the mass flow rate, the supersonic part of the flow is not incorporated in the optimization program. Another program for simulation of individual flow problems does incorporate the supersonic flow and a normal shock. The shock equations were taken from Shapiro [7]. Non

<sup>1</sup>The velocity of sound is defined as  $a = \sqrt{\{\partial p / \partial \rho\}_s}$ . With (eq.4) which leads to  $M = v/a = v/\sqrt{\rho/\gamma p} = v/\sqrt{\gamma R T}$  for ideal gases.

<sup>2</sup>Transition from supersonic to subsonic flow without the occurrence of shock waves is even under laboratory conditions hard to achieve (Leijdens [2]). They are certainly not common in leakage flows.

normal shocks are typically multi-dimensional and therefore they cannot be represented in a one-dimensional model.

## OPTIMIZATION ALGORITHM

Peveling presents his results as charts of the flow coefficient versus the pressure ratio. The latter is defined as the mass flow rate compared by a theoretical value which is computed according to<sup>3</sup>:

$$\dot{m}_{\text{theoretic}} = A \rho_0 \Pi^{-1/\gamma} \sqrt{\frac{2\gamma}{\gamma-1} R T_0 (1 - \Pi^{(1-\gamma)/\gamma})}$$

Here  $\Pi$  is the ratio of the inlet and the outlet pressure ( $\Pi > 1$ ),  $A$  is the minimal flow area and the index 0 denotes inlet conditions. Choking and thereby the maximum mass flow rate, is assumed when the pressure ratio exceeds a critical value:

$$\Pi_{\text{critical}} = \left( \frac{2}{\gamma+1} \right)^{\gamma/(1-\gamma)}$$

Before optimization can start, a well defined criterium for the performance is required. It should be a function of the parameters in the optimization only (here  $a$  and  $b$  from (eq.1)). The criterium goes by the name of object function. In this case the root mean square of the deviation of the flow coefficients of 24 computed conditions, denoted by  $\alpha_i(a, b)$  ( $i$  indexes the condition), from the measured ( $\alpha_i$ ) is used:

$$f_{\text{obj}}(a, b) = \sqrt{\frac{1}{N} \sum_{i=1}^N (\alpha_i(a, b) - \alpha_i)^2} \quad \text{with} \quad N = 24$$

The 24 points are taken from the experiments by Peveling [6] (shortly described in the parallel paper) and are tabulated in figure 2.

pressure ratio	flow coefficients			
	clearance in mm			
1.2	0.76	0.84	1.01	1.12
1.4	0.78	0.87	0.90	0.99
1.6	0.79	0.85	0.93	0.94
1.8	0.79	0.85	0.93	0.94
2.0	0.81	0.86	0.93	0.95
2.2	0.83	0.87	0.94	0.95

Figure 2: The 24 conditions taken from Peveling's experimental data and used within the object function.

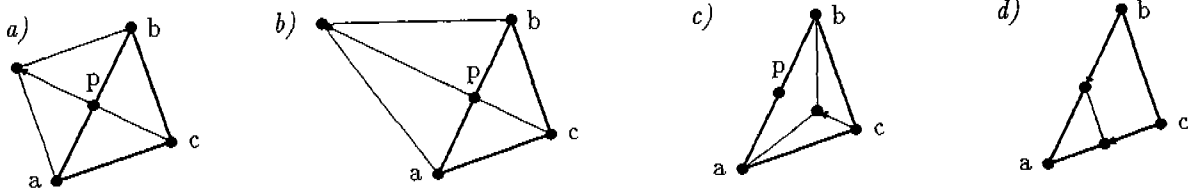


Figure 3: The Downhill Simplex Method: When vertex  $c$  has the worst performance, it is manipulated according to: a) Reflection in the center of gravity of the remaining vertices, denoted  $p$ . b) When the result is even better than the best vertex so far, elongation away from the center of gravity is attempted. c) When a) did not lead to any improvement, contraction of  $c$  towards the center of gravity is tried. d) When all fails the entire simplex is contracted towards the best vertex (here  $a$ ). It can be shown that by repeating this sequence the simplex always converges to an optimum.

The Downhill Simplex Method for optimization is described by Press *et al* [3]. A simplex is the mathematical concept of  $N + 1$  points or vertices in an  $N$  dimensional space together with their interconnecting line segments, faces, *etc.* In the two dimensional case (here the  $a, b$ -space) this leads to a triangle, in three dimensions it would

<sup>3</sup>The theoretical mass flow rate is based on the integral formulation of the energy equation for isentropic flow of a perfect gas, by neglecting the inlet velocity and assuming the outlet pressure coincides with the pressure in the throat. The latter assumption is a rather crude simplification.

be a tetrahedron (not necessarily regular). For each point the value of the object function is computed to assign a performance parameter to it. By manipulation, as shown in fig.3, the simplex converges around a minimum of the object function. Press *et al* use, with a sense of humor, the term *amoeba* for the deforming, walking triangle.

# RESULTS

The output of the optimization program consists of the optimal values for  $a$  and  $b$  and the flow coefficients for the 24 conditions specified above. The latter are listed in figure 4 and shown in figure 5 together with the simulation of Ishii's experiments in the same way as described in the parallel paper. For the coefficients was found:

$$a = 0.247 \quad b = -0.276$$

Comparison of the graphs in figure 5 with similar graphs in the parallel paper reveals a far better agreement for the experiments by Peveling. This was expected since the model is optimized for these. The agreement with Ishii is still not very good, though a slight improvement is found. The mass flow rate proved to be proportional to the pressure ratio for  $\Pi \geq 2$ .

pressure ratio	flow coefficients			
	clearance in mm			
	0.10	0.15	0.20	0.50
1.2	0.75	0.87	0.97	1.22
1.4	0.79	0.89	0.95	1.02
1.6	0.81	0.87	0.90	0.96
1.8	0.82	0.86	0.88	0.94
2.0	0.82	0.86	0.89	0.94
2.2	0.82	0.86	0.89	0.94

Figure 4: The flow coefficients computed with the optimized shear stress model for the 24 conditions used during the optimization.

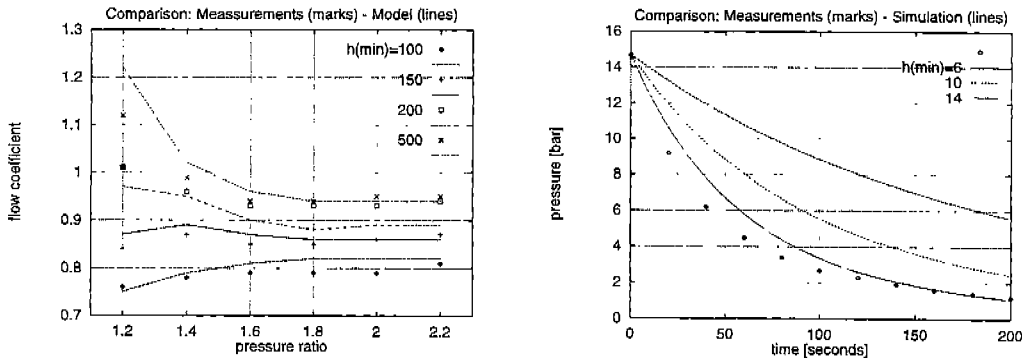


Figure 5: Comparison of the predicted flow coefficients for Peveling's experiments (left) and the pressure-time curve of Ishii's (right). The legends give the clearance in  $\mu\text{m}$ .

# Behavior of the Flow

Figure 6 shows the conditions for Peveling's experiments that are predicted to choke. For the experiments by Ishii the critical pressure ratio at which choking should occur is about ten percent lower than for Peveling's conditions ( $\Pi = 1.75$  versus  $\Pi = 1.89$ ). But the predictions of the flow model only give choking from  $\Pi = 1.2$  and only for the highest clearance (14  $\mu\text{m}$ ). The reason is that the viscous effects, which are much larger in the much more narrow channel of Ishii, suppress the acceleration. This is confirmed by the results of figure 6 which show that choking gets more likely as the clearance increases.

Figure 7 clearly shows this effect in the flow properties. The sonic point moves downstream as a result of the viscosity and the shock upstream. As a result the shock loses much of its strength.

pressure ratio	clearance in mm			
	0.10	0.15	0.20	0.50
1.2	○	○	○	●
1.4	○	○	○	●
1.6	○	●	●	●
1.8	●	●	●	●
2.0	●	●	●	●
2.2	●	●	●	●

Figure 6: Classification of the conditions of the experiments by Peveling: choking (●) or fully subsonic (○) flow.

The limitation of the model as explained just below (eq.5) is encountered a few times for both experiments. They occur for pressure ratio's just above critical.

## CONCLUSIONS

The optimization of the wall shear stress modeling for quasi one-dimensional steady state models for gas leakage proved to be worth while. The newly proposed model is:  $\xi = a \cdot Re^b$  with  $a = 0.247$  and  $b = -0.276$ .

The predicted mass flow rates, for the experiments on which the optimization was based, is much more realistic than with the model of Blasius. The new model also gives a slight improvement for experiments which differ in fluidum, pressure ratio's and geometry. Although this is not fully satisfactory, it is ground for some confidence in the model. There is a physical limitation to the model: under some conditions the flow is either unstable or shows multi dimensional effects. The results also show that choking and therefore shock waves, are likely to occur in relative wide channels.

Finally the linear proportional relation between the mass flow rate and the pressure ratio, as suggested in the parallel paper is supported by the new results. Only in the low pressure ratio range ( $\Pi < 2$ ) the results divert from this relation.

Two-dimensional computations based on commercial CFD software are scheduled for future research. By solving the velocity profile the semi-empirical relation for the friction coefficient becomes superfluous. Though these types of computations are too time consuming for thermodynamic simulation of screw compressors, it might lead to more insight and further improvement of one-dimensional models.

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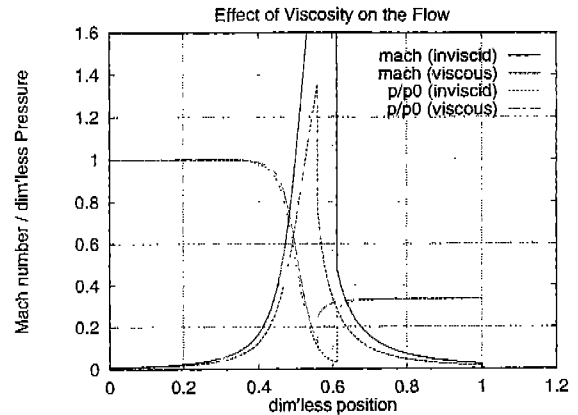


Figure 7: The effect of viscosity on supersonic flow: the sonic point moves down stream and the shock upstream.